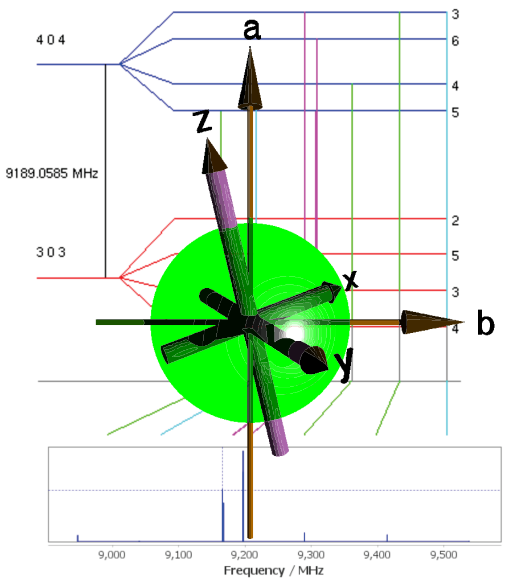
EXPLAINER: EFFECTS OF NUCLEAR QUADRUPOLE COUPLING TENSOR MAGNITUDE, ASYMMETRY, AND ORIENTATION ON THE APPEARANCE OF ROTATIONAL HYPERFINE STRUCTURE

S. A. COOKE, *Natural and Social Science, Purchase College SUNY, Purchase, NY, USA*.

Towards easier high resolution spectral assignment for asymmetric molecules bearing nuclei with spins greater than $\frac{1}{2}$ a systematic study has been performed examining how different nuclear quadrupole coupling (NQC) tensors cause different hyperfine patterns. The asymmetry of the NQC tensors principal components, the overall magnitudes of the components, and the orientation of the NQC tensor principal axes with respect to the molecular principal axes are considered from the perspective of directly *observable* rotational transition splittings. Effects of different molecular asymmetry are also considered. Also, while $I = \frac{3}{2}$ is the nuclear spin most thoroughly investigated, different nuclear spins are also examined. The SPCAT/SPFIT software has been used to simulate many thousands of spectra with the goal of identifying recognizable patterns which will be presented.



Thoughts concerning the incorporation of this material into the undergraduate curriculum will be presented together with a reflection on the statement "*An electrostatic field gradient is a classical quantity and presents no conceptual problem to the undergraduate student in their first year; nuclear quadrupole coupling constants can thus be introduced quite early...*"[a].

[a] *Nuclear Quadrupole Coupling Constants*, E. A. C. Lucken, Academic Press Inc. New York, New York, 1969